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Aspects of Quantum Field Theory in Curved Space-Time

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Chapter 1
A Quick Course in Quantum Mechanics

This book is concerned with the quantum theory of fields satisfying linear equations of motion. As a prerequisite, one needs to understand the quantum theory of particles, which is related to field theory as finite-dimensional linear algebra is related to functional analysis. In particular, we need to treat the simplest linear quantum system, the harmonic oscillator.

Classical mechanics: The canonical formalism

The dynamics of a typical mechanical system is described by a system of second-order ordinary differential equations, the *Newtonian equations of motion*:

$$\frac{d^2\mathbf{x}}{dt^2} = \mathbf{F}\left(\mathbf{x}, \frac{d\mathbf{x}}{dt}, t\right). \tag{1.1}$$

Often the force $\mathbf{F}$ is the negative of the gradient of a *potential* function, $V(\mathbf{x})$. In the simplest situation, $\mathbf{x}(\cdot)$ is a function from $\mathbf{R}$ (the domain of the time variable) to $\mathbf{R}^d$ (the *configuration space* of the system), where d equals $3n$ for a system of n particles in the real world of dimension 3. (More generally, $\mathbf{R}^d$ may be replaced by some other manifold, and the time may need to be restricted to a subinterval of $\mathbf{R}$, but such complications are not relevant to our present concerns.)

Let $\dot{\mathbf{x}} \equiv d\mathbf{x}/dt$. Suppose that (1.1) arises as the Euler–Lagrange equation of a problem in the calculus of variations: to extremize the *action functional*

$$S \equiv \int_{t_1}^{t_2} L\big(\mathbf{x}(t), \dot{\mathbf{x}}(t), t\big)\, dt.$$

L is called the *Lagrangian* of the system. The functions $\mathbf{x}$ which extremize S satisfy

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}^j}\right) = \frac{\partial L}{\partial x^j} \qquad (j = 1, \ldots, d). \tag{1.2}$$

These are the *Lagrangian equations of motion.*

For example, from the Lagrangian (with $d = 1$)

$$L = \tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}m\omega^2 x^2$$

we obtain $\frac{d}{dt}(m\dot{x}) = -m\omega^2 x$, which is equivalent to the Newtonian equation

$$\ddot{x} + \omega^2 x = 0.$$

This system is the one-dimensional *harmonic oscillator* of mass m and frequency ω; if $\omega = 0$ it becomes a free particle (in one dimension), and if ω^2 is replaced by a negative number, one has a "runaway" particle (the solutions being exponential).

The *canonical momentum conjugate to* x^j is

$$p_j \equiv \frac{\partial L}{\partial \dot{x}^j}\,.$$

The *Hamiltonian* is defined by

$$H \equiv -L + \dot{x}^j p_j\,,$$

where a sum over j is understood. For the harmonic oscillator, for example, we have $p = m\dot{x}$ and $H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2$. In the more general class of problems usually studied in quantum mechanics,

$$H = \frac{1}{2m}\,\mathbf{p}^2 + V(\mathbf{x}).$$

H can be interpreted as the energy of the physical system, but its main significance for the general formulation of mechanics lies elsewhere: Let us regard H as a function of $\mathbf{x}$ and $\mathbf{p}$ (rather than of $\mathbf{x}$ and $\dot{\mathbf{x}}$). (This is a *Legendre transformation*; a mathematically precise reference on Legendre transformations (in a different context) is Maslov & Fedoriuk 1981, Sec. 1.3.) Then (1.2) is easily seen to be equivalent to the *Hamiltonian equations of motion*,

$$\frac{dx^j}{dt} = +\frac{\partial H}{\partial p_j}\,, \qquad \frac{dp_j}{dt} = -\frac{\partial H}{\partial x^j}\,. \tag{1.3}$$

Phase space is $\mathbf{R}^{2d}$ with the coordinates $(\mathbf{x}, \mathbf{p})$. (More generally, the phase space is the cotangent bundle of the manifold which serves as

configuration space; $\mathbf{p}(t)$ is a cotangent vector and $\dot{\mathbf{x}}(t)$ a tangent vector at the point $\mathbf{x}(t)$. This accounts for the placement of the index on x and $\dot{x}$ as a superscript.) Thus, the second-order differential system (1.1) or (1.2) has been replaced by a first-order system, (1.3), in a space of twice the dimension. A *pure state* of a classical system is a point in phase space (as opposed to an impure or mixed state, which is a probability distribution on phase space). An *observable* is just a function of $\mathbf{x}$ and $\mathbf{p}$. We measure the observable $A(\mathbf{x}, \mathbf{p})$ simply by "looking" at the system and observing A to have its value at the point of phase space where the system happens to be! By measuring $2d$ independent observables, such as $\mathbf{x}$ and $\mathbf{p}$ themselves, exactly and simultaneously, we completely determine the state.

Quantum states and observables

In microscopic physics, observations are inherently probabilistic. A *pure state* of a quantum system is a one-dimensional subspace of a complex Hilbert space, $\mathcal{H}$. The subspace is traditionally represented by one of the vectors in it, normalized (i.e., $\|\Psi\| = 1$). Ψ is determined by the state only up to phase, but one speaks informally of "the state Ψ" when there is no chance of confusion. An *observable* is represented by a self-adjoint operator in $\mathcal{H}$. Often the operator is unbounded, and hence its domain is a dense subspace of $\mathcal{H}$, not the whole space. When the observable A is measured, its *expectation value* is

$$\langle A \rangle = \langle \Psi, A\Psi \rangle \equiv \langle \Psi | A | \Psi \rangle. \tag{1.4}$$

The fundamental postulate of the physical interpretation of quantum theory is that the average of the results of many experiments to measure A on identical systems under identical conditions is given by the formula (1.4).

Notational remarks: The middle member of (1.4) is an inner product in $\mathcal{H}$, reexpressed in the last member in *Dirac notation*. I use the conventions standard in physics, wherein the complex conjugate of a number z is denoted z^* (not $\overline{z}$), and the adjoint of a matrix or operator A is $A^\dagger$ (not A^*). Furthermore, the inner product is linear in the *right* variable, not the left:

$$\langle \Psi, z\Phi \rangle = z \langle \Psi, \Phi \rangle, \quad \langle z\Psi, \Phi \rangle = z^* \langle \Psi, \Phi \rangle.$$

In the Dirac notation, where $\langle \Psi, \Phi \rangle \equiv \langle \Psi | \Phi \rangle$, the angular brackets are thought of as permanently attached to the vectors; thus "$|\Phi\rangle$" is a typical element of $\mathcal{H}$, and "$\langle \Psi|$" is the linear functional defined by taking the inner product of the argument vector with Ψ. (By the Riesz theorem, all linear functionals on $\mathcal{H}$ (elements of the dual space of $\mathcal{H}$) are of this form.)

As a first example, consider a purely canonical system, where $\mathcal{H} = \mathcal{L}^2(\mathbf{R}^d)$. That is, the vectors are complex-valued, square-integrable functions $\Psi(\mathbf{x})$ (the famous "wave functions"). The operator representing the position observable x^j is simply multiplication by the variable x^j. The observable p_j is represented by the operator $-i\,\partial/\partial x^j$, in appropriate units (that is, units in which Planck's constant, $\hbar$, equals 1 — which I shall always use).

This system has an alternative description by functions $\hat{\Psi}(\mathbf{p})$. Now the momentum observable is represented by multiplication by p_j, and the position by $+i\,\partial/\partial p_j$. $\hat{\Psi}$ is just the Fourier transform of Ψ; these two distinct square-integrable functions are two different representations of the same vector in the abstract Hilbert space of physical states.

A more complicated example is presented by a (nonrelativistic) particle of spin $\frac{1}{2}$. In this case the Hilbert space is $\mathcal{L}^2(\mathbf{R}^3) \oplus \mathcal{L}^2(\mathbf{R}^3)$. That is, the vectors are *pairs* of square-integrable functions, $\Psi_a(\mathbf{x})$ ($a = 1$ or 2). In addition to $\mathbf{x}$ and $\mathbf{p}$, there are some fundamental observables of the theory which are represented by matrices acting on the index a (leaving $\mathbf{x}$ alone):

$$S_1 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S_2 = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad S_3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

These observables are the components of the particle's spin, or intrinsic angular momentum, in the three directions of physical space. They have no counterpart in the classical phase-space formalism.

The *commutator* of two operators is

$$[A, B] \equiv AB - BA.$$

In the examples, the commutators of the basic observables are

$$[x^j, p_k] = i\delta^j_k$$

and

$$[S_1, S_2] = iS_3$$

with its cyclic permutations; also, the various components of $\mathbf{x}$ or of $\mathbf{p}$ commute among themselves, and the positions and momenta commute with the spins. If $[A, B] \neq 0$, then A and B can't be measured simultaneously. (Here "measured" means not only that a certain numerical value is experimentally obtained, but also that the physical system is left in such a state that the identical value would with certainty be obtained if the measurement were repeated immediately.) That is, states characterized by "sharp" values of A necessarily have spread-out probability distributions for measurements of B. A pure state can, at best, be characterized by the values of "a complete set of commuting observables", not of *all* observables.

If these commuting observables all have totally discrete spectra, then there is a orthonormal basis for $\mathcal{H}$ whose elements are labelled by their possible eigenvalues. (This is what it means for the set to be "complete".) That is, if the set comprises, say, three observables, $\{A_1, A_2, A_3\}$, then there are vectors $|\alpha_1, \alpha_2, \alpha_3\rangle$ (for each α_j in the spectrum $\sigma(A_j)$) such that

$$A_1|\alpha_1, \alpha_2, \alpha_3\rangle = \alpha_1|\alpha_1, \alpha_2, \alpha_3\rangle, \qquad \text{etc.},$$

and for any normalized $\Psi \in \mathcal{H}$,

$$\Psi = \sum_{\alpha_j \in \sigma(A_j)} \psi(\alpha_1, \alpha_2, \alpha_3)|\alpha_1, \alpha_2, \alpha_3\rangle,$$

$$\sum_{\alpha_j \in \sigma(A_j)} |\psi(\alpha_1, \alpha_2, \alpha_3)|^2 = 1.$$

Finally, $|\psi(\alpha_1, \alpha_2, \alpha_3)|^2$ is the probability of finding A_j to have the value α_j when the three observables are simultaneously measured.

If continuous spectra occur, we can no longer speak of basis vectors, but the representation of Ψ by a coefficient function ψ is still valid. For example, the spin-$\frac{1}{2}$ particle has a complete commuting set $\{x^1, x^2, x^3, S_3\}$, and the wave function $\Psi_a(\mathbf{x}) \equiv \psi(\mathbf{x}, a) \in \mathcal{L}^2(\mathbf{R}^3) \oplus \mathcal{L}^2(\mathbf{R}^3)$ is the representation of a state relative to that choice of basic observables. (An alternative choice might be $\{x^1, p_2, p_3, S_1\}$.) Also,

$$\sum_{a=1}^{2} \int_V |\psi(\mathbf{x}, a)|^2 \, d^3x$$

is the probability that the particle will be found to be in the set $V \subset \mathbf{R}^3$ with either of the allowed values $(\pm\frac{1}{2})$ of S_3.

Note that an equation of motion is inadequate to specify a quantum system. We must also know what the observable operators are. In many cases the commutation relations essentially uniquely determine the operators. More precisely, the abstract algebra defined by the commmutation relations has a unique irreducible representation up to unitary equivalence. For example, the *Stone–Von Neumann theorem* for the canonical commutation relation, $[x, p] = i$, and its *finite-dimensional* generalizations state that (under technical assumptions which are not entirely innocent, since they eliminate the elementary example of "a particle in a box") the only quantum system supporting those commutation relations is the one built on the Hilbert space $\mathcal{L}^2(\mathbf{R}^d)$ as described above. (See, for instance, Putnam 1967, Chap. 4.) In other elementary cases the contrary is true, however. For instance, the two-dimensional (spin $\frac{1}{2}$) representation is only one of the infinite sequence of representations of the SU(2) Lie algebra, $[S_1, S_2] = iS_3$ etc. Different spin representations represent *different physical systems* (different kinds of particle), rather than different states of a single system. Although quantum field theory, as we'll see, can be regarded as an infinite-dimensional generalization of the canonical commutation relations, the Stone–Von Neumann theorem does not apply there, and inequivalent representations do exist. (See Segal 1967, and Wightman 1967, Secs. 6–7.) (That is, there are distinct sets of operators satisfying the commutation relations; these sets are *essentially* different, not transformable into one another by recoordinatizations of the Hilbert space like the Fourier transform of $\mathcal{L}^2(\mathbf{R}^d)$.) Therefore, the passage from a formal algebra of observables to a full quantum theory in a Hilbert space is a very nontrivial step in field theory. Apart from the thorny technical problems, the choice of a physically appropriate representation is a major conceptual issue, especially in the context of curved space-time. In field theory the inequivalent representations can sometimes represent different physical configurations of the same system, although by no means are all representations physically meaningful.

Quantum dynamics: The Heisenberg picture

Quantum field theory is usually developed in the *Heisenberg picture*, a formulation in which the operators satisfy equations of motion

like those of the classical observable quantities they represent.

Let us solve the equation of motion of the harmonic oscillator,

$$\ddot{x} + \omega^2 x = 0,$$

with *operator initial data.* Because of the linearity of the equation, this can be done by simply writing down the standard general solution and interpreting the arbitrary constants in it as operators. We have

$$x(t) = x(0)\cos\omega t + \frac{1}{\omega}\,\dot{x}(0)\sin\omega t, \tag{1.5}$$

where $\dot{x}(0) = p(0)/m$. (When $\omega = 0$, this reduces to

$$x(t) = x(0) + \frac{p(0)}{m}\,t, \tag{1.6}$$

which classically is the trajectory of a free particle.) The derivative of (1.5), times m, provides a formula for $p(t)$. At $t = 0$ we take the canonical operators to have their usual (*Schrödinger*) representation, discussed above:

$$x(0) = x \quad \text{(the multiplication operator)}, \qquad p(0) = -i\,\frac{\partial}{\partial x}\,. \tag{1.7}$$

Then (1.5) defines $x(t)$ and $p(t)$ for each $t \in \mathbf{R}$ as operators in $\mathcal{L}^2(\mathbf{R})$. It is easy to see that they satisfy the canonical relation, $[x,p]\big|_t = i$.

By the Stone–Von Neumann theorem, these operators are unitarily equivalent to those in (1.6); I shall exhibit later the unitary operator connecting them. However, they are quite distinct as concrete operators in the space of wave functions, $\mathcal{L}^2$. The physical interpretation of this situation is that $\langle\Psi|x(t)|\Psi\rangle$ and $\langle\Psi|p(t)|\Psi\rangle$ are the expectation values of the position and momentum if those quantities were to be measured at time t with the particle in the state Ψ. The state itself is a time-independent concept (at least so long as the system evolves under its internal dynamics, without interaction with external agencies). The state Ψ is an abstract object in a Hilbert space, $\mathcal{H}$. It is *represented* by a function $\Psi(x) \in \mathcal{L}^2$; this representation has been arbitrarily chosen to be the one which gives directly the probability density for position measurements at $t = 0$. The probability densities for momentum measurements and for position measurements at other times are given similarly in other representations; in this one, at least the expectation

values for such measurements can be calculated from (1.5), using the concrete form of the inner product, $\langle \Psi, \Phi \rangle = \int_{-\infty}^{\infty} \Psi(x)^* \Phi(x)\, dx$.

It is interesting to note that (when ω is defined as I have done) the classical equation of motion is independent of the mass, m, but different values of m denote physically different *quantum* systems: The relation between $\dot{x}$ and p depends on m, and hence so will the expected results of measurements of x at later times, for a given initial wave function. On the other hand, m may be eliminated from the formalism by redefining x to absorb a factor $\sqrt{m}$. To concentrate attention on the ω dependence, I henceforth set $m = 1$.

Let's treat the harmonic oscillator in the Hamiltonian approach. Recall that we have $H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$ and hence from (1.3) the equations of motion

$$\frac{dx}{dt} = p, \qquad \frac{dp}{dt} = -\omega^2 x.$$

We shall solve this by the method of *creation and annihilation operators*: Let

$$x = \frac{1}{\sqrt{\omega}}(a + a^\dagger), \qquad p = -i\sqrt{\omega}(a - a^\dagger), \tag{1.8}$$

so that

$$a \equiv \frac{1}{2}\left(\omega^{\frac{1}{2}} x + i\omega^{-\frac{1}{2}} p\right), \qquad a^\dagger = \frac{1}{2}\left(\omega^{\frac{1}{2}} x - i\omega^{-\frac{1}{2}} p\right).$$

(Classically all these quantities are complex numbers, and $a^\dagger$ is simply a^*. In quantum mechanics, x and p are self-adjoint operators, so $a^\dagger$ is indeed the adjoint of the operator a — at least if we ignore technicalities about the domains of unbounded operators.) It is easy to see that the equations of motion become

$$\frac{d}{dt}a = -i\omega a, \qquad \frac{d}{dt}a^\dagger = +i\omega a^\dagger,$$

with solution

$$a(t) = e^{-i\omega t}\, a(0), \qquad a(t)^\dagger = e^{+i\omega t}\, a(0)^\dagger.$$

We then arrive at

$$\begin{aligned} x(t) &= \frac{1}{\sqrt{\omega}}\left[a(0)e^{-i\omega t} + a(0)^\dagger e^{i\omega t}\right], \\ p(t) = \dot{x}(t) &= -i\sqrt{\omega}\left[a(0)e^{-i\omega t} - a(0)^\dagger e^{i\omega t}\right], \end{aligned} \tag{1.9}$$

which are equivalent to (1.5).

This construction is the prototype of the quantization of a field theory satisfying a linear, time-independent equation of motion. Note, however, that it does not apply to the case $\omega = 0$, where the definition of a breaks down. Nor does it apply when ω^2 is replaced by a negative number. As we'll soon see, it is through the annihilation-creation operators that the notion of "particles" enters the formalism. We must therefore be prepared to encounter situations where the particle concept is not applicable. If our most fundamental model of nature is a field theory, then we are saying that fields are more fundamental than particles.

Now consider a more general quantum-mechanical system, corresponding to equations of motion which are time-independent (autonomous) but not necessarily linear. Ordinarily it is assumed that there is a self-adjoint *Hamiltonian operator*, H, such that the equation of motion for each observable operator is equivalent to

$$\frac{dA}{dt} = i[H, A]. \tag{1.10}$$

This is the *Heisenberg equation of motion.* This much can be true even for a time-dependent dynamics, in which case H is a function of time as well as of the basic observables of the theory. If H is independent of time, however, the solution of the Heisenberg equation can be written

$$A(t) = U(t)^{-1} A(0) U(t), \qquad U(t) \equiv e^{-itH}.$$

$U(t)$ is a unitary operator, so $U(t)^{-1} = U(t)^\dagger = e^{+itH}$.

In purely canonical cases, H is obtained from the classical Hamiltonian function on phase space, $H(\mathbf{x}, \mathbf{p})$, by substituting $-i\,\partial/\partial x^j$ for p_j and interpreting x^j as a multiplication operator. This prescription makes elementary sense in the Schrödinger representation as long as H is polynomial in its dependence on $\mathbf{p}$, and one can then verify that

$$i[H, x^j] = \frac{\partial H}{\partial p_j}, \qquad i[H, p_j] = -\frac{\partial H}{\partial x^j},$$

as needed for consistency of (1.10) and (1.3).

Advanced remarks: Nonpolynomial terms in $H(\mathbf{x}, \mathbf{p})$ may be interpreted via the Fourier transformation (if the term is independent

of $\mathbf{x}$) or the calculus of pseudodifferential operators [Petersen 1983, Treves 1980, Taylor 1981]. However, there is an *ordering ambiguity*: Since the operators x and p don't commute, it is unclear whether the classical function x^2p^2 should be interpreted as $\frac{1}{2}(x^2p^2+p^2x^2)$ or xp^2x or $\frac{1}{2}(xpxp+pxpx)$ or something else. (Since the operator should be formally self-adjoint, one can at least restrict attention to expressions with palindromic symmetry, as I have here.) Consequently, there are in principle *many* quantum systems corresponding to a given classical system; their Hamiltonians differ by terms involving the canonical commutator, $[x,p]=\hbar i$, and the presence of $\hbar$ (in general units) indicates why such terms should disappear in the classical limit. H. Weyl's attempt at a resolution of this ambiguity [Weyl 1927; Moyal 1949] was a precursor of what is now called the *Weyl calculus for pseudodifferential operators* [Grossmann *et al.* 1968; Hörmander 1979]. Such issues can be ignored in elementary quantum mechanics, because the Hamiltonians of most physical systems are quadratic in $\mathbf{p}$ with quadratic term independent of $\mathbf{x}$. (An $\mathbf{x}$-dependent linear term is not considered to present a problem: $f(\mathbf{x})\mathbf{p}$ is interpreted in the first way that comes to mind, $\frac{1}{2}(f\mathbf{p}+\mathbf{p}f)$.)

The Schrödinger picture

The nonrelativistic quantum mechanics of particles is usually conducted in a different formalism, where the operator representing an observable A is the same at all times, while the *states* evolve. (This *Schrödinger picture* is not the same thing as the "Schrödinger [or position] representation", which is a particular realization of the states as wave functions.) The equation of motion of the states is the *(time-dependent) Schrödinger equation*,

$$i\frac{\partial\Psi}{\partial t}=H\Psi.$$

In a purely canonical theory with H polynomial in $\mathbf{p}$, this is a linear partial differential equation. For example, for the harmonic oscillator (with $m=1$) it is

$$i\frac{\partial\Psi(x,t)}{\partial t}=-\frac{1}{2}\frac{\partial^2\Psi}{\partial x^2}+\frac{1}{2}\omega^2x^2\Psi.$$

In most cases of interest the linear partial differential operator H is of the *elliptic* type; by hypothesis, it is self-adjoint.

When H is independent of t, the solution of the initial-value problem for the Schrödinger equation is

$$\Psi(t) = e^{-itH}\,\Psi(0).$$

What this means in concrete terms is that the equation can be solved by separation of variables: If one looks for solutions of the form $\Psi(t,x) = \psi(x)T(t)$, one finds that $T(t) = e^{-iEt}$ and

$$H\psi = E\psi$$

for some number E. (This is called the *time-independent Schrödinger equation.*) Therefore, the problem reduces, in principle, to finding the eigenvectors of the self-adjoint operator H, or, more generally, the spectral representation of H:

Suppose, first, that H possesses a complete set of eigenvectors $\{\psi_j\}$,

$$H\psi_j = E_j\psi_j, \qquad \|\psi_j\| = 1.$$

Then the initial data for the Schrödinger equation can be expanded as

$$\Psi(0) = \sum_{j=1}^{\infty} c_j\psi_j, \qquad c_j = \langle\psi_j|\Psi(0)\rangle.$$

(In the Schrödinger representation the ψ_j will be functions of $\mathbf{x}$, and the coefficients have the formula $c_j = \int \psi_j(\mathbf{x})^*\Psi(0,\mathbf{x})\,d^dx$.) Therefore,

$$\Psi(t) = \sum_{j=1}^{\infty} c_j\psi_j e^{-iE_jt} \equiv e^{-itH}\Psi(0). \tag{1.11}$$

If H has continuous spectrum, then the solutions of the partial differential equation $H\psi = E\psi$ generally are not square-integrable and hence are not vectors in $\mathcal{H} = \mathcal{L}^2(\mathbf{R}^d)$. Nevertheless, at least in simple cases one can complete the classical procedure of solution by separation of variables to obtain the general solution as an integral over such solutions, regarded as "generalized eigenvectors". (This construction provides a concrete realization of the abstract *spectral theorem*, which generalizes the eigenvector expansion to deal with the most general self-adjoint operators.) We delay a detailed discussion to Chapter 2, and consider a few fundamental examples here.

Example 1: **The free particle in three-dimensional space.** The time-independent Schrödinger equation is the Helmholtz equation,

$$H\psi \equiv -\frac{1}{2m}\nabla^2\psi = E\psi.$$

Its basic solutions are

$$\psi_{\mathbf{k}}(\mathbf{x}) \equiv e^{i\mathbf{k}\cdot\mathbf{x}}, \qquad E = \frac{k^2}{2m}$$

($k \equiv |\mathbf{k}|$). It follows that the general solution of the time-dependent equation is

$$\Psi(t,\mathbf{x}) = (2\pi)^{-\frac{3}{2}} \int_{\mathbf{R}^3} d^3k\, e^{i\mathbf{k}\cdot\mathbf{x}}\, e^{-k^2t/2m}\, \hat{\psi}(\mathbf{k}),$$

where

$$\hat{\psi}(\mathbf{k}) \equiv (2\pi)^{-\frac{3}{2}} \int_{\mathbf{R}^3} d^3x\, e^{-i\mathbf{k}\cdot\mathbf{x}}\, \Psi(0,\mathbf{x}).$$

Thus the eigenfunction expansion in this case is the Fourier transform (and we refer to the general theory of the Fourier transform to justify the normalization factors $(2\pi)^{-\frac{3}{2}}$).

Since $(\mathbf{p}\psi)\hat{}\,(\mathbf{k}) = \mathbf{k}\,\hat{\psi}(\mathbf{k})$, what we have really done here is to pass to a representation of the Hilbert space in which the momentum observable, $\mathbf{p}$, is diagonal. The three components of $\mathbf{p}$ make up the complete set of commuting observables. But since E is a function of $\mathbf{p}$ in this problem, we can also regard the eigenfunction expansion as an integral over E, supplemented by an integration over the angles in $\mathbf{k}$-space:

$$\begin{aligned}(2\pi)^{-\frac{3}{2}} \int d^3k &= (2\pi)^{-\frac{3}{2}} \int_0^\infty k^2\, dk \int_0^{2\pi} d\phi_{\mathbf{k}} \int_0^\pi \sin\theta_{\mathbf{k}}\, d\theta_{\mathbf{k}} \\ &\equiv \int d\mu(E) \int d\Omega_{\mathbf{k}},\end{aligned}$$

where, since $k = \sqrt{2mE}$, we calculate that $d\mu(E) = (2\pi)^{-\frac{3}{2}} m^{\frac{3}{2}} \times \sqrt{2E}\, dE$. Returning momentarily to the general problem, we anticipate in analogy with this example an eigenfunction expansion with the schematic structure

$$\Psi(t,\mathbf{x}) = \int_{\sigma(H)} d\mu(E) \sum_\alpha c_\alpha(E)\, e^{-iEt}\, \psi_{E,\alpha}(\mathbf{x}).$$

Here α is the eigenvalue of another observable that goes together with H to make a complete commuting set, or an n-tuple of eigenvalues of a set of such observables. The summation range of α may depend on E, and, as the example shows, α may itself be a continuous variable. (The notation has been chosen to make this equation a generalization of the discrete eigenfunction expansion (1.11), but in terms of a notation used earlier in this chapter, $\psi_{E,\alpha}$ is $|E, \alpha_2, \dots\rangle$ and $c_\alpha(E)$ is $\psi(E, \alpha_2, \dots)$.) In general, "$\int_{\sigma(H)} d\mu(E)$" entails a summation over discrete eigenvalues of H and an integration over the continuous spectrum of H; thus μ is a Stieltjes measure with support in $\sigma(H)$, the spectrum of H. As the example of a free particle shows, even when the spectrum is completely (and, for the experts, absolutely) continuous, it may be convenient to normalize the measure as something different from the Lebesgue measure.

Example 2: **The harmonic oscillator.** With $m = 1$, the equation is

$$H\psi \equiv -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}\omega^2 x^2 \psi = E\psi.$$

I summarize two well known methods of solving this problem (Messiah 1961, Chap. 12 and App. B3).

The first method is to solve the differential equation directly in terms of known special functions. The square-integrable eigenfunctions are

$$\psi_n(x) \equiv N_n\, H_n(\sqrt{\omega}x)\, e^{-\omega x^2/2},$$

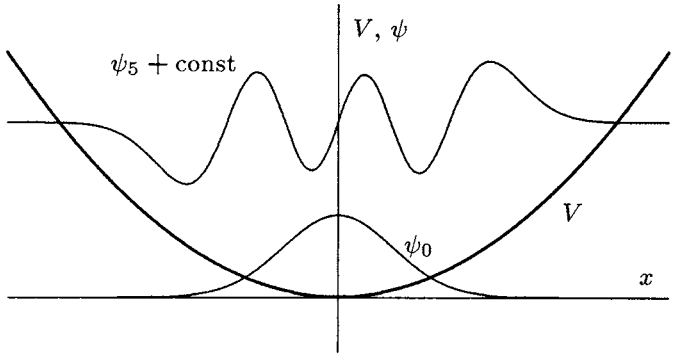
with eigenvalues

$$E_n = \left(n + \tfrac{1}{2}\right)\omega, \qquad n = 0,\ 1,\ 2,\ \dots.$$

H_n is the *Hermite polynomial* of degree n, and N_n is a certain normalization constant. This operator has a discrete spectrum; (1.11) applies. The nth eigenfunction has $n - 1$ nodes (zeros), and it is oscillatory in the region where E_n exceeds the potential, exponentially decaying outside that region. The figure shows the potential ($V \equiv \frac{1}{2}\omega^2 x^2$) and two typical eigenfunctions, one of them raised on the graph for clarity.

The second method is an algebraic trick peculiar to this potential. In studying the oscillator in the Heisenberg picture, we introduced the non-self-adjoint operator

$$a = \frac{1}{2}\left(\omega^{\frac{1}{2}} x + i\omega^{-\frac{1}{2}} p\right).$$



A bit of calculation shows

$$[a, a^\dagger] = 1, \qquad H = \omega a^\dagger a + \tfrac{1}{2}\omega.$$

Define

$$N \equiv a^\dagger a.$$

Then we find that

$$Na = a(N-1), \qquad Na^\dagger = a^\dagger(N+1).$$

Now suppose we have a vector $|n\rangle$ ($n \in \mathbf{R}$) such that $N|n\rangle = n|n\rangle$. Then

$$Na|n\rangle = (n-1)a|n\rangle, \qquad Na^\dagger|n\rangle = (n+1)a^\dagger|n\rangle.$$

That is, $a|n\rangle$ and $a^\dagger|n\rangle$, if they are not zero, are also eigenvectors of N. Also, we find that the square of the norm of $a|n\rangle$ is

$$\langle n|a^\dagger a|n\rangle = n\,\langle n|n\rangle.$$

Therefore, n must be nonnegative. Furthermore, if $n = 0$, then $a|n\rangle = 0$, and conversely (whereas $a^\dagger|n\rangle \neq 0$ always). By induction, n must be a nonnegative integer, since the sequence of eigenvalues corresponding to the vectors of the form $a \cdots a|n\rangle$ is not allowed to jump over 0. Starting from $|0\rangle$, we can construct the normalized eigenvectors

$$|n\rangle = \frac{1}{\sqrt{n!}}\,(a^\dagger)^n\,|0\rangle.$$

(Do not confuse $|0\rangle$ with 0, the zero vector in the Hilbert space!) The action of the creation and annihilation operators on these basis vectors is

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle, \qquad a|n\rangle = \sqrt{n}\,|n-1\rangle.$$

We have found a Hilbert space (the closed span of the orthonormal basis $\{|n\rangle\}$) in which the operators x, p, and H act with their correct commutation relations. Each of these operators is actually self-adjoint and hence has a spectral representation; in the representation where x acts diagonally, $|n\rangle$ is identified with the Hermite function $\psi_n(x)$ previously discussed. The spectral representation of H is, of course, the one we are looking at, since H is manifestly diagonal here. One thinks of $|n\rangle$ as representing a state in which n "excitations" or "quanta" are present. N counts such excitations, $a^\dagger$ creates them, and a destroys them. Apart from the constant term $\frac{1}{2}\omega$, the energy (eigenvalue of H) is proportional to n. *This construction is the prototype for the introduction of particles into quantum field theory.* Particles are merely excitations of a field.

If the Hilbert space spanned by $\{|n\rangle\}$ is not the entire Hilbert space of the system, then any eigenvector of H linearly independent from it would, by the same argument, yield another copy of the whole sequence of eigenvectors. This would mean that the representation of x and p is not irreducible; there are additional, independent observables in the theory. For example, a spin-$\frac{1}{2}$ oscillator's Hilbert space is the direct sum of two copies of this elementary oscillator space, with basis $\{|n, \pm\rangle\}$; and a two-dimensional oscillator's space is the direct product, with basis $\{|n_1, n_2\rangle\}$.

Of course, there are some gaps in this argument. How (without appealing to the Stone–Von Neumann theorem) does one exclude the possibility of a representation in which N has continuous spectrum? Or the possibility that some steps in the argument are meaningless because a vector is not in the domain of the unbounded operator that is applied to it?

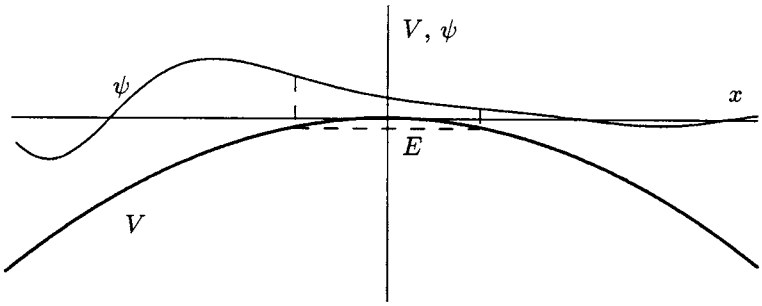
Nevertheless, this example illustrates that the formal algebra of commutation relations can carry one a long way. It even separates the main features of the model system from irrelevant details of special-function theory.

Example 3: **The repulsive oscillator.** The Hamiltonian

$$H = \tfrac{1}{2}p^2 - \tfrac{1}{2}\omega^2 x^2$$

classically describes an exponentially runaway particle. Titchmarsh 1962, Theorem 5.10, shows that H is essentially self-adjoint (i.e., defines a self-adjoint operator in $\mathcal{L}^2(\mathbf{R})$ without the aid of extra boundary

conditions at infinity), and that $\sigma(H) = (-\infty, \infty)$. (The spectrum is continuous and is unbounded below.) The figure shows the potential and a typical eigenfunction (a parabolic cylinder function plotted from data in the National Bureau of Standards Handbook (Abramowitz & Stegun 1968)). Note the transitions from exponential to oscillatory behavior where the potential crosses the energy of the eigenfunction (a small negative number in this case).



Models such as this, with arbitrarily negative energy, are in physical disrepute. The idea is that the slightest perturbation of the dynamics would introduce a coupling between the repulsive oscillator and the other, normal degrees of freedom of the world. If such an object existed, therefore, there would be a dynamical instability in which the energy of the runaway particle tumbled to an arbitrarily low value while the energy of the rest of the world grew without bound. Thus, the predictions of such a theory could not be physically plausible. If an H of this sort arose by linearization of some physically realistic theory, one would expect that the neglected nonlinear interactions actually halt the runaway motion and stabilize the system. The linearized theory would therefore be a bad approximation to the full theory. Nevertheless, field theories with inverted-oscillator potentials are amusing to contemplate and raise some important issues about quantization procedures and the relation between fields and particles (see the appendix).

The connection between the two pictures

If H is independent of t, the solution of the Schrödinger equation, $i\,\partial\Psi/\partial t = H\Psi$, can be written

$$\Psi(t,x) = U(t)\Psi(0,x), \qquad U(t) \equiv e^{-itH}.$$

One can *redefine* the state vectors and operators by a time-dependent similarity transformation:

$$\tilde{\Psi} \equiv U(t)^{-1}\Psi(t), \qquad \tilde{A}(t) \equiv U(t)^{-1}AU(t).$$

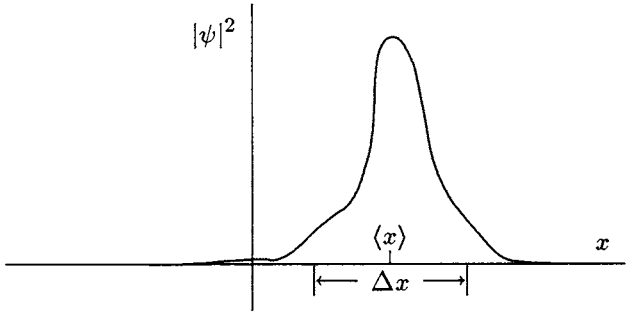
Then the new state vector is independent of time, while the observable operators evolve according to the Heisenberg picture. All the matrix elements $\langle\Psi|A|\Phi\rangle$, hence all physical predictions of the theory, are unchanged.

If H depends on t, then the quantum dynamics is given by a two-parameter family of operators, $U(t_2, t_1)$, rather than the one-parameter Lie group, $U(t_2 - t_1) = e^{-i(t_2-t_1)H}$. (In the Schrödinger picture, for example, $U(t_2, t_1)$ maps initial data at t_1 to the wave function at time t_2.) In quantum theories with finitely many degrees of freedom, one can still use these operators to move back and forth between Heisenberg and Schrödinger pictures. In quantum field theory, however, especially with a time-dependent dynamical law, the very *existence* of a U (or an H, or a Schrödinger picture) is not a foregone conclusion.

The classical limit

Under what circumstances do we get classical behavior from a (canonical) quantum system? Let us consider a particle of mass m in one dimension. For the details see Messiah 1961, Chap. 6; see also Maslov & Fedoriuk 1981 for a different aspect of the question. The essential conclusions can be carried over to field systems (at least to bosonic ones).

The important question is: What are the ratios of the characteristic lengths of the situation at hand?



(1) For a classical description of the position to be meaningful, the wave function $\psi(x)$ must be sharply peaked about its mean or expectation value, $\langle x \rangle$. That is,

$$\Delta x \equiv \left\langle (x - \langle x \rangle)^2 \right\rangle^{\frac{1}{2}}$$

must be small compared to lengths of experimental significance.

(2) If we demand *localization in phase space*, not just in configuration space, then we must also have Δp small compared to momenta of experimental significance. Here, however, we must accept the implications of the celebrated *uncertainty principle*, which in this context is a theorem of classical Fourier analysis in $\mathcal{L}^2(\mathbf{R})$:

$$(\Delta x)(\Delta p) \geq \frac{1}{2} \quad \text{for any } \psi.$$

Therefore, the product of the "experimentally significant" units of x and p must be sufficiently large for the classical picture of the system to be valid.

(3) Let's suppose that we don't care about measuring p for its own sake. We still want a classical description of x over a significant time interval. From (1.6),

$$\Delta x(t) = \Delta x(0) + \frac{\Delta p}{m} t.$$

So to keep Δx small we must keep $\frac{t}{m\Delta x}$ small. (For the harmonic oscillator, from (1.5), we must keep $(m\omega\Delta x)^{-1}$ small.) In particular, this means that potentially classical behavior is associated with *large* m. This classical limit *of systems*, $m \to \infty$, is nonuniform in t — and also nonuniform in the state ψ, as described by Δx and Δp.

Parallel to the mathematician's sensitivity to nonuniform convergence is the physicist's dictum that only limits of *dimensionless parameters* have intrinsic significance. The classical limit of quantum theory is often said to be the limit $\hbar \to 0$, but $\hbar$ is a red herring. One can always choose units where $\hbar$ equals 1. In fact, to do otherwise distracts attention from the genuine small parameters in the problem at hand — which are ratios of $\hbar$ to other quantities with the dimensions of action (length × momentum, or energy × time) — and from the accompanying nonuniformities in the limit. (Nevertheless, taking $\hbar$ to zero is a